Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1201txs

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	14	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	15	APR 04	EMBASE - Database reloaded and enhanced

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 19:08:48 ON 15 APR 2005

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 19:08:57 ON 15 APR 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8
DICTIONARY FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

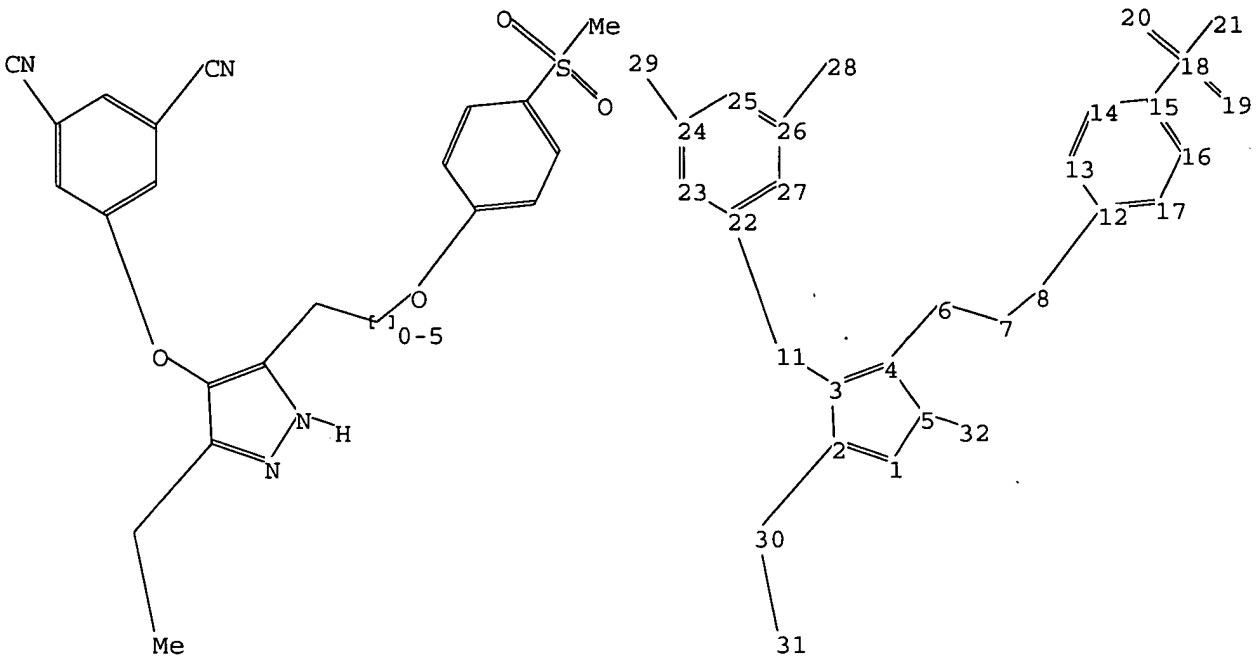
Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10657033.str



chain nodes :
6 7 8 11 18 19 20 21 28 29 30 31 32
ring nodes :
1 2 3 4 5 12 13 14 15 16 17 22 23 24 25 26 27
chain bonds :
2-30 3-11 4-6 5-32 6-7 7-8 8-12 11-22 15-18 18-19 18-20 18-21 24-29
26-28 30-31
ring bonds :
1-2 1-5 2-3 3-4 4-5 12-13 12-17 13-14 14-15 15-16 16-17 22-23 22-27
23-24 24-25 25-26 26-27
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 7-8 8-12 11-22 15-18 18-19 18-20
exact bonds :
2-30 4-6 5-32 6-7 18-21 24-29 26-28 30-31
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17 22-23 22-27 23-24 24-25 25-26 26-27

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS
30:CLASS 31:CLASS 32:CLASS

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 19:09:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS

```
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:             0 TO        0
PROJECTED ANSWERS:                0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 ful
FULL SEARCH INITIATED 19:09:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      3 TO ITERATE

100.0% PROCESSED       3 ITERATIONS                          1 ANSWERS
SEARCH TIME: 00.00.01

L3            1 SEA SSS FUL L1

=> d l3 ibib hitstr abs
'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
are:  (RN = CAS Registry Number)

REG    - RN
SAM    - Index Name, MF, and structure - no RN
FIDE   - All substance data, except sequence data
IDE    - FIDE, but only 50 names
SQIDE  - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD    - Protein sequence data, includes RN
SQD3   - Same as SQD, but 3-letter amino acid codes are used
SQN    - Protein sequence name information, includes RN

CALC   - Table of calculated properties
EPROP  - Table of experimental properties
PROP   - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance.  The substance formats
must be cited first.  The CA File predefined formats are:

ABS  -- Abstract
APPS -- Application and Priority Information
BIB  -- CA Accession Number, plus Bibliographic Data
CAN  -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND  -- Index Data
IPC  -- International Patent Classification
PATS -- PI, SO
STD  -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
```

ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):0
'0' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.76	161.97

FILE 'CAPLUS' ENTERED AT 19:09:57 ON 15 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 1 L3

=> d his

(FILE 'HOME' ENTERED AT 19:08:48 ON 15 APR 2005)

FILE 'REGISTRY' ENTERED AT 19:08:57 ON 15 APR 2005
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 1 S L1 FUL

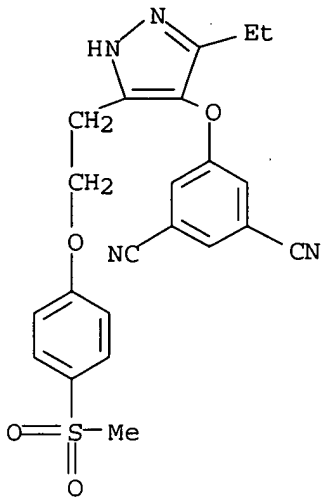
FILE 'CAPLUS' ENTERED AT 19:09:57 ON 15 APR 2005
L4 1 S L3

=> d l4 ibib hitstr abs

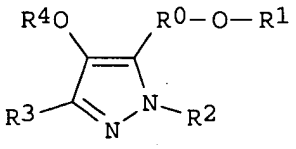
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:308421 CAPLUS
DOCUMENT NUMBER: 140:321351
TITLE: Preparation of pyrazole derivatives as therapeutic agents for HIV mediated diseases
INVENTOR(S): Edwards, Paul John; Jones, Lyn Howard; Mowbray, Charles Eric; Stupple, Paul Anthony; Tran, Isabelle
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031156	A1	20040415	WO 2003-IB4214	20030924
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005054707	A1	20050310	US 2003-657033	20030905
PRIORITY APPLN. INFO.:			GB 2002-23234 A	20021007

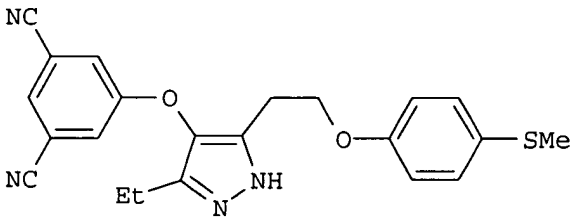
OTHER SOURCE(S): MARPAT 140:321351
IT **678992-82-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)
RN 678992-82-0 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



GI



I



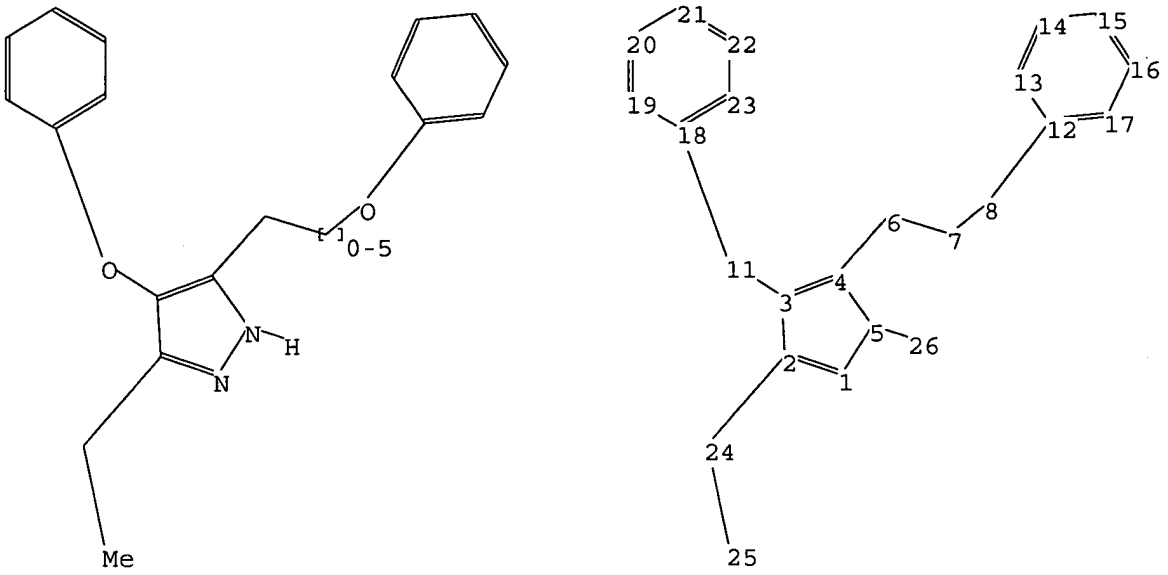
II

AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are useful in the treatment of a variety of disorders including those in which the inhibition' of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodificiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-{[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     6.29     168.26

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -0.73      -0.73

FILE 'REGISTRY' ENTERED AT 19:11:28 ON 15 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   14 APR 2005  HIGHEST RN 848555-82-8
DICTIONARY FILE UPDATES:  14 APR 2005  HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\106570331.str
```



chain nodes :
6 7 8 11 24 25 26
ring nodes :
1 2 3 4 5 12 13 14 15 16 17 18 19 20 21 22 23
chain bonds :
2-24 3-11 4-6 5-26 6-7 7-8 8-12 11-18 24-25
ring bonds :
1-2 1-5 2-3 3-4 4-5 12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23
19-20 20-21 21-22 22-23
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 7-8 8-12 11-18
exact bonds :
2-24 4-6 5-26 6-7 24-25
normalized bonds :
12-13 12-17 13-14 14-15 15-16 16-17 18-19 18-23 19-20 20-21 21-22 22-23

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS

L5 STRUCTURE UPLOADED

=> s l5
SAMPLE SEARCH INITIATED 19:11:48 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80

PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s l5 ful
FULL SEARCH INITIATED 19:11:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 21 TO ITERATE

100.0% PROCESSED 21 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

L7 7 SEA SSS FUL L5

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	329.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.73

FILE 'CAPLUS' ENTERED AT 19:12:03 ON 15 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l6
L8 0 L6

=> s l7
L9 2 L7

=> d l9 ibib hitstr abs

L9 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:308421 CAPLUS
DOCUMENT NUMBER: 140:321351
TITLE: Preparation of pyrazole derivatives as therapeutic agents for HIV mediated diseases
INVENTOR(S): Edwards, Paul John; Jones, Lyn Howard; Mowbray,

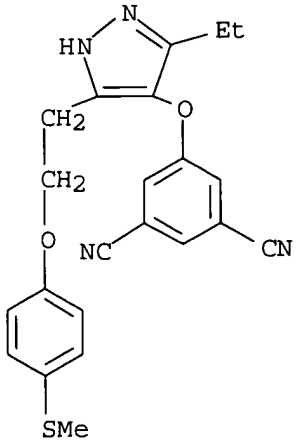
Charles Eric; Stupple, Paul Anthony; Tran, Isabelle
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031156	A1	20040415	WO 2003-IB4214	20030924
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005054707	A1	20050310	US 2003-657033	20030905
PRIORITY APPLN. INFO.:			GB 2002-23234 A	20021007

OTHER SOURCE(S): MARPAT 140:321351

IT **678992-80-8P 678992-83-1P 678992-84-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

RN 678992-80-8 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylthio)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



RN 678992-83-1 CAPLUS
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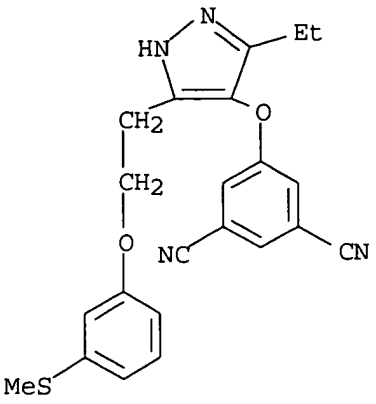

RN 678992-84-2 CAPLUS
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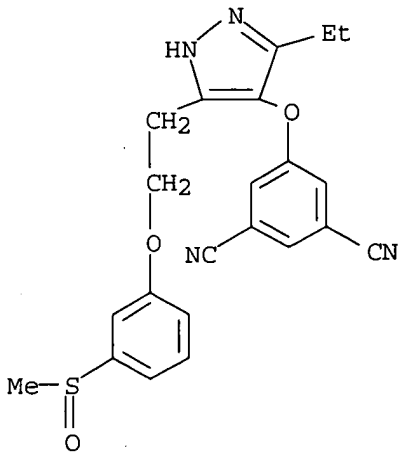
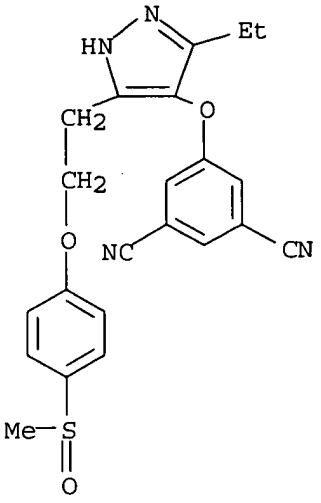
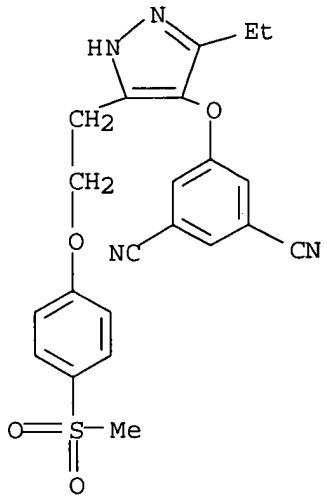


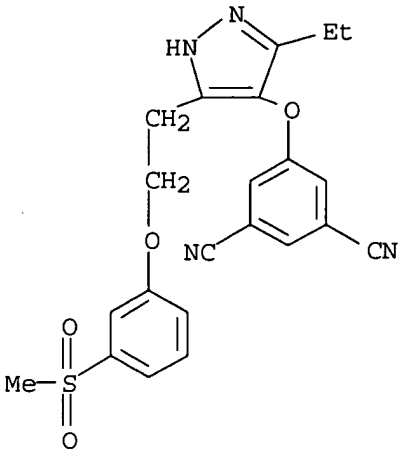
IT **678992-81-9P 678992-82-0P 678992-85-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)
RN 678992-81-9 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylsulfinyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



RN 678992-82-0 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



RN 678992-85-3 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[3-(methylsulfonyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



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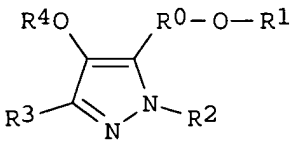

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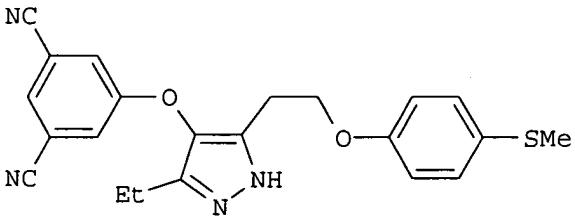


II

AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are useful in the treatment of a variety of disorders including those in which the inhibition' of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodificiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-{[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

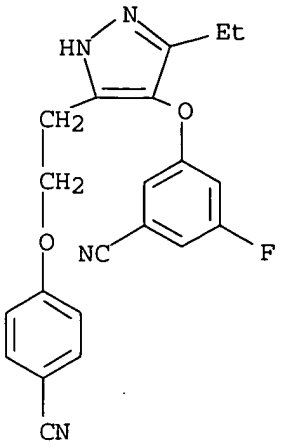
=> d l9 ibib hitstr abs 2

L9 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:832763 CAPLUS
DOCUMENT NUMBER: 137:337884
TITLE: Preparation of aryloxy pyrazole derivatives as reverse transcriptase inhibitors for treating HIV
INVENTOR(S): Jones, Lyn Howard; Mowbray, Charles Eric; Price, Davis Anthony; Selby, Matthew Duncan; Stupple, Paul Anthony
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085860	A1	20021031	WO 2002-IB1234	20020404
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2443449	AA	20021031	CA 2002-2443449	20020404
EP 1377556	A1	20040107	EP 2002-708600	20020404
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EE 200300497	A	20040216	EE 2003-497	20020404
BR 2002008811	A	20040309	BR 2002-8811	20020404
JP 2004531535	T2	20041014	JP 2002-583387	20020404
US 2003100554	A1	20030529	US 2002-118512	20020405
ZA 2003007095	A	20040910	ZA 2003-7095	20030910
NO 2003004523	A	20031209	NO 2003-4523	20031009

PRIORITY APPLN. INFO.:	GB 2001-8999	A	20010410
	GB 2001-27426	A	20011115
	US 2001-289570P	P	20010508
	US 2002-346727P	P	20020107
	WO 2002-IB1234	W	20020404

OTHER SOURCE(S): MARPAT 137:337884
IT **473921-42-5P**, 3-[[5-[2-(4-Cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluorobenzonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)
RN 473921-42-5 CAPLUS
CN Benzonitrile, 3-[[5-[2-(4-cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



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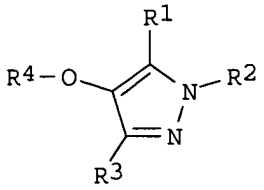

I

AB This invention relates to pyrazole derivs. (shown as I; e.g. 2-Amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone) or pharmaceutically acceptable salts, solvates or derivative thereof, wherein R1 to R4 are defined below, and to processes for the preparation thereof, intermediates used in their preparation of, compns. containing them and the uses of such derivs. The compds. of the present invention bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof. As such the compds. of the present invention are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). In tests of inhibition of HIV-1 reverse transcriptase enzyme, the claimed compds. 2-amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone, 3,5-dimethyl-4-[[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]benzonitrile and 1-(3-azetidinyl)-4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazole had IC50 values of 39,000, 3,200 and 248 nM, resp. In I: R1 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R10, -CONR5R10, R8 or R9. R2 is H, C1-C6 alkyl, C3-C6 alkenyl, C3-C6 alkynyl, C3-C7 cycloalkyl, C3-C7 cycloalkenyl, Ph, benzyl, R8 or R9; or, R1 and R2, when taken together, represent unbranched C3-C4 alkylene. R3 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R5, -CONR5R5, R8 or R9; R4 is Ph, naphthyl or pyridyl. Definitions of R5 and R7-R10 and addnl. specifications are given in the claims. Included are 283 claimed-compound

prepns. and 115 intermediate prepns.
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	12.58	342.17

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.46	-2.19

FILE 'REGISTRY' ENTERED AT 19:15:28 ON 15 APR 2005

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8
DICTIONARY FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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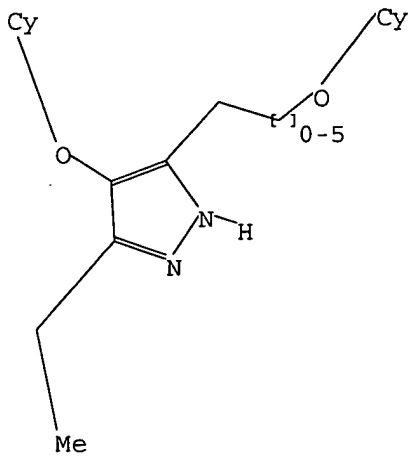
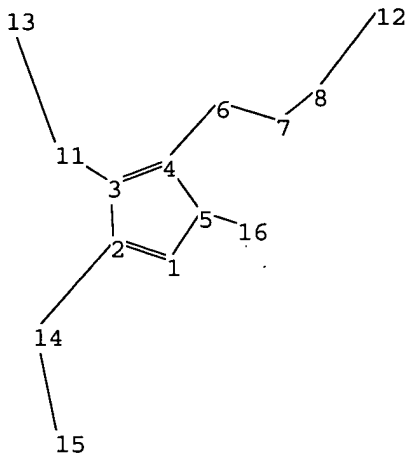
Uploading C:\Program Files\Stnexp\Queries\106570332.str





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6 7 8 11 12 13 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
2-14 3-11 4-6 5-16 6-7 7-8 8-12 11-13 14-15
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 7-8 8-12 11-13
exact bonds :
2-14 4-6 5-16 6-7 14-15

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS

L10 STRUCTURE UPLOADED

=> s l10
SAMPLE SEARCH INITIATED 19:15:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 24 TO ITERATE

100.0% PROCESSED 24 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 187 TO 773
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=> s l10 ful
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FULL SCREEN SEARCH COMPLETED - 645 TO ITERATE

100.0% PROCESSED 645 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.01

L12 10 SEA SSS FUL L10

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	503.50

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.19

FILE 'CAPLUS' ENTERED AT 19:16:04 ON 15 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l12
L13 2 L12

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	503.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.19

FILE 'CAPLUS' ENTERED AT 19:16:16 ON 15 APR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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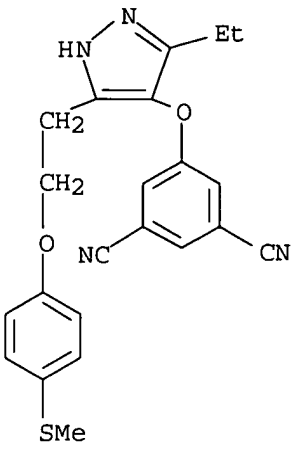
L14 2 L12

=> d l14 ibib hitstr abs

L14 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:308421 CAPLUS
DOCUMENT NUMBER: 140:321351
TITLE: Preparation of pyrazole derivatives as therapeutic agents for HIV mediated diseases
INVENTOR(S): Edwards, Paul John; Jones, Lyn Howard; Mowbray, Charles Eric; Stupple, Paul Anthony; Tran, Isabelle
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031156	A1	20040415	WO 2003-IB4214	20030924
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005054707	A1	20050310	US 2003-657033	20030905
PRIORITY APPLN. INFO.:			GB 2002-23234 A	20021007

OTHER SOURCE(S): MARPAT 140:321351
IT **678992-80-8P 678992-83-1P 678992-84-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)
RN 678992-80-8 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylthio)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



RN 678992-83-1 CAPLUS
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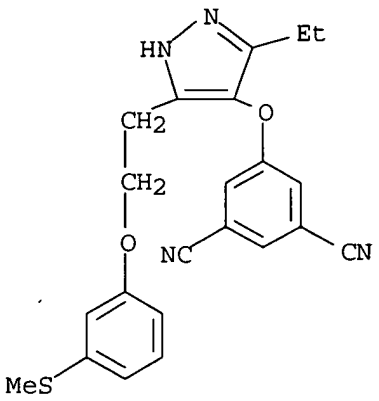

RN 678992-84-2 CAPLUS
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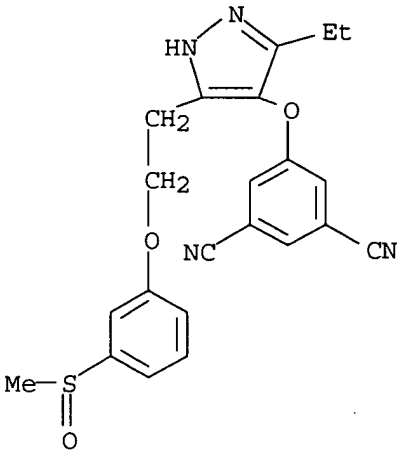

IT **678992-81-9P 678992-82-0P 678992-85-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

RN 678992-81-9 CAPLUS
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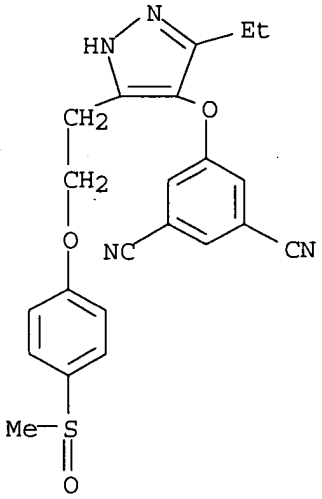

RN 678992-82-0 CAPLUS
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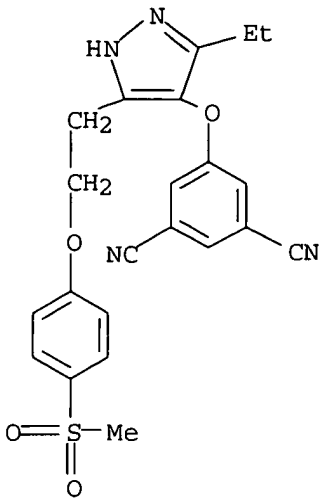

RN 678992-85-3 CAPLUS
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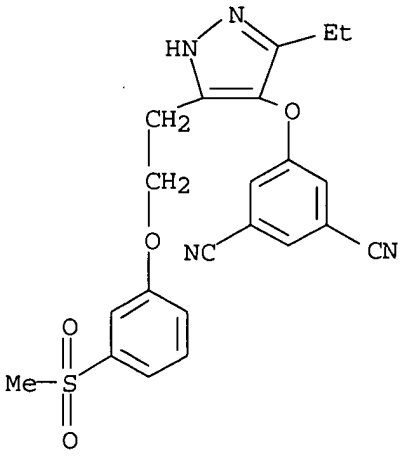

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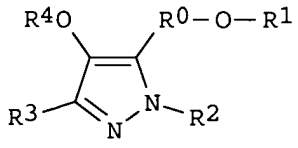

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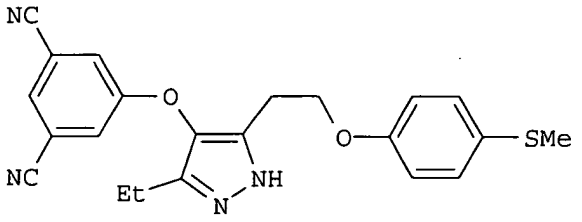

II

AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are useful in the treatment of a variety of disorders including those in which the inhibition' of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodificiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-{[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l14 ibib hitstr abs 2

L14 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:832763 CAPLUS
DOCUMENT NUMBER: 137:337884
TITLE: Preparation of aryloxy pyrazole derivatives as reverse transcriptase inhibitors for treating HIV
INVENTOR(S): Jones, Lyn Howard; Mowbray, Charles Eric; Price, Davis Anthony; Selby, Matthew Duncan; Stupple, Paul Anthony
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085860	A1	20021031	WO 2002-IB1234	20020404
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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EP 1377556	A1	20040107	EP 2002-708600		20020404
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
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US 2003100554	A1	20030529	US 2002-118512		20020405
ZA 2003007095	A	20040910	ZA 2003-7095		~~20030910~~
NO 2003004523	A	20031209	NO 2003-4523		20031009
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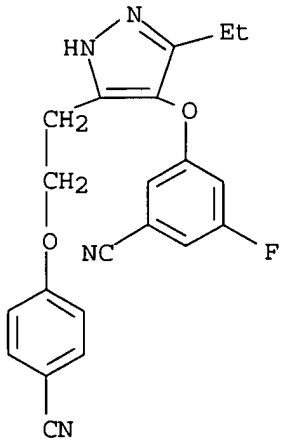
			GB 2001-27426	A	20011115
			US 2001-289570P	P	20010508
			US 2002-346727P	P	20020107
			WO 2002-IB1234	W	20020404

OTHER SOURCE(S): MARPAT 137:337884

IT **473921-42-5P**, 3-[[5-[2-(4-Cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluorobenzonitrile **473921-43-6P**, 3-Fluoro-5-[[3-ethyl-5-(2-((2-methyl-3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile **473921-44-7P**, 3-Fluoro-5-[[3-ethyl-5-(2-((3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile **473921-45-8P**, 3-Fluoro-5-[[3-ethyl-5-(2-((2-amino-3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)

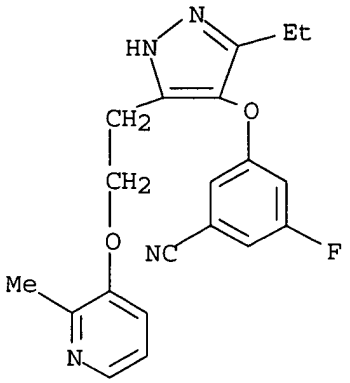
RN 473921-42-5 CAPLUS

CN Benzonitrile, 3-[[5-[2-(4-cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)

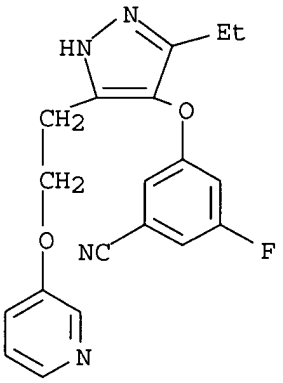


RN 473921-43-6 CAPLUS

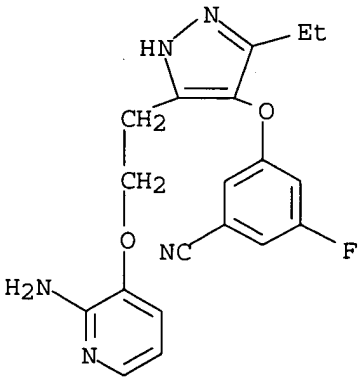
CN Benzonitrile, 3-[[3-ethyl-5-[2-[(2-methyl-3-pyridinyl)oxy]ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



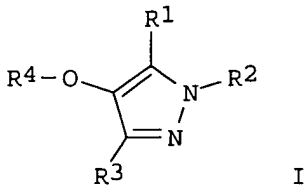
RN 473921-44-7 CAPLUS
CN Benzonitrile, 3-[[3-ethyl-5-[2-(3-pyridinyloxy)ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 473921-45-8 CAPLUS
CN Benzonitrile, 3-[[5-[2-[(2-amino-3-pyridinyl)oxy]ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



GI



I

AB This invention relates to pyrazole derivs. (shown as I; e.g. 2-Amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone) or pharmaceutically acceptable salts, solvates or derivative thereof, wherein R1 to R4 are defined below, and to processes for the preparation thereof, intermediates used in their preparation of, compns. containing them and the uses of such derivs. The compds. of the present invention bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof. As such the compds. of the present invention are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). In tests of inhibition of HIV-1 reverse transcriptase enzyme, the claimed compds. 2-amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone, 3,5-dimethyl-4-[[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]benzonitrile and 1-(3-azetidinyl)-4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazole had IC50 values of 39,000, 3,200 and 248 nM, resp. In I: R1 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R10, -CONR5R10, R8 or R9. R2 is H, C1-C6 alkyl, C3-C6 alkenyl, C3-C6 alkynyl, C3-C7 cycloalkyl, C3-C7 cycloalkenyl, Ph, benzyl, R8 or R9; or, R1 and R2, when taken together, represent unbranched C3-C4 alkylene. R3 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R5, -CONR5R5, R8 or R9; R4 is Ph, naphthyl or pyridyl. Definitions of R5 and R7-R10 and addnl. specifications are given in the claims. Included are 283 claimed-compound prepns. and 115 intermediate prepns.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	12.58	516.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.46	-3.65

FILE 'REGISTRY' ENTERED AT 19:19:48 ON 15 APR 2005
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STRUCTURE FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8
DICTIONARY FILE UPDATES: 14 APR 2005 HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

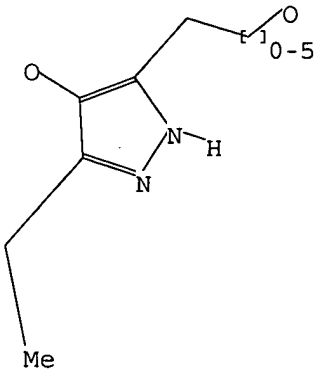
Please note that search-term pricing does apply when conducting SmartSELECT searches.

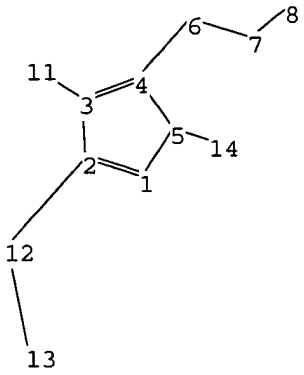
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\106570333.str





chain nodes :
6 7 8 11 12 13 14
ring nodes :
1 2 3 4 5
chain bonds :
2-12 3-11 4-6 5-14 6-7 7-8 12-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 3-4 3-11 4-5 7-8
exact bonds :
2-12 4-6 5-14 6-7 12-13

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS

```
L15     STRUCTURE UPLOADED

=> s l15
SAMPLE SEARCH INITIATED 19:20:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     24 TO ITERATE

100.0% PROCESSED      24 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          187 TO      773
PROJECTED ANSWERS:               0 TO        0

L16         0 SEA SSS SAM L15

=> s l15 ful
FULL SEARCH INITIATED 19:20:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    645 TO ITERATE

100.0% PROCESSED     645 ITERATIONS                              14 ANSWERS
SEARCH TIME: 00.00.01

L17          14 SEA SSS FUL L15

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   161.33     677.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -3.65

FILE 'CAPLUS' ENTERED AT 19:20:20 ON 15 APR 2005
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FILE COVERS 1907 - 15 Apr 2005  VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005  (20050414/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.
```

```
=> s l17
L18           2 L17

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     3.15     681.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -3.65

FILE 'REGISTRY' ENTERED AT 19:24:21 ON 15 APR 2005
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STRUCTURE FILE UPDATES:   14 APR 2005  HIGHEST RN 848555-82-8
DICTIONARY FILE UPDATES:  14 APR 2005  HIGHEST RN 848555-82-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\106570334.str
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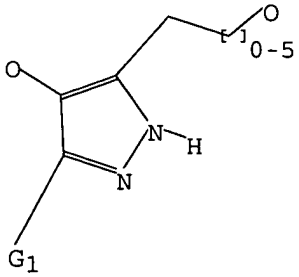

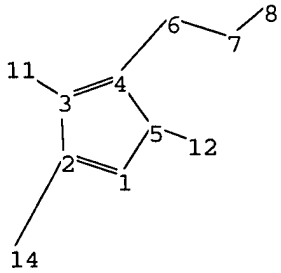

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chain nodes :
6  7  8  11  12  14
ring nodes :
1  2  3  4  5
chain bonds :
2-14  3-11  4-6  5-12  6-7  7-8
ring bonds :
1-2  1-5  2-3  3-4  4-5
exact/norm bonds :
1-2  1-5  2-14  3-11  4-5  7-8
exact bonds :
2-3  3-4  4-6  5-12  6-7
isolated ring systems :
containing 1 :


G1:C,H,O,X,Cb,Ak,CN

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  11:CLASS
12:CLASS  14:CLASS



L19     STRUCTURE UPLOADED

=> s l19
SAMPLE SEARCH INITIATED 19:24:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    105 TO ITERATE

100.0% PROCESSED     105 ITERATIONS                              2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1486 TO     2714
PROJECTED ANSWERS:               2 TO      124

L20           2 SEA SSS SAM L19

=> s l19 ful
FULL SEARCH INITIATED 19:24:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   2368 TO ITERATE

100.0% PROCESSED    2368 ITERATIONS                             63 ANSWERS
SEARCH TIME: 00.00.01

L21          63 SEA SSS FUL L19

=> file caplus
COST IN U.S. DOLLARS                              SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                 161.33     842.34

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                   0.00      -3.65
```

FILE 'CAPLUS' ENTERED AT 19:24:56 ON 15 APR 2005
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 15 Apr 2005 VOL 142 ISS 17
FILE LAST UPDATED: 14 Apr 2005 (20050414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l21
L22 24 L21

=> d l24 ibib hitstr abs 1-24
L24 NOT FOUND
The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> d l22 ibib hitstr abs 1-24

L22 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:308421 CAPLUS
DOCUMENT NUMBER: 140:321351
TITLE: Preparation of pyrazole derivatives as therapeutic agents for HIV mediated diseases
INVENTOR(S): Edwards, Paul John; Jones, Lyn Howard; Mowbray, Charles Eric; Stupple, Paul Anthony; Tran, Isabelle
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031156	A1	20040415	WO 2003-IB4214	20030924

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2005054707 A1 20050310 US 2003-657033 20030905

PRIORITY APPLN. INFO.: GB 2002-23234 A 20021007

OTHER SOURCE(S): MARPAT 140:321351

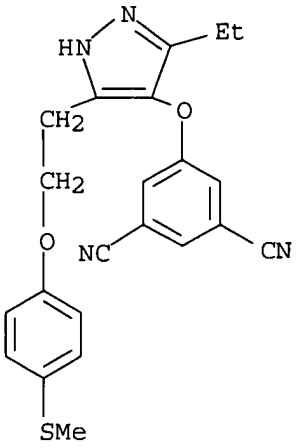
IT **678992-80-8P 678992-83-1P 678992-84-2P**

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

RN 678992-80-8 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylthio)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



RN 678992-83-1 CAPLUS

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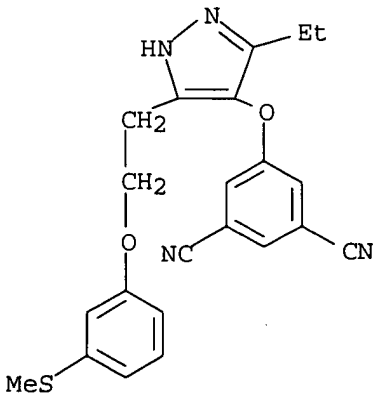
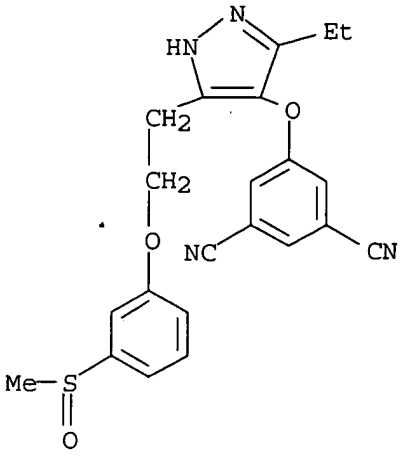


RN 678992-84-2 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[3-(methylsulfinyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX

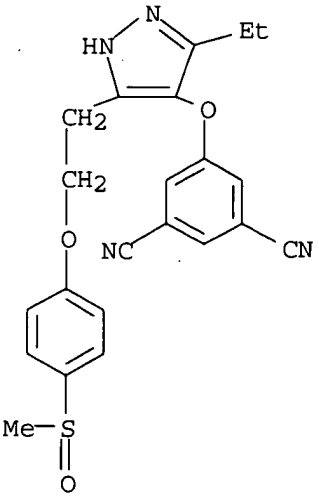
NAME)



IT **678992-81-9P 678992-82-0P 678992-85-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)

RN 678992-81-9 CAPLUS

CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-[4-(methylsulfinyl)phenoxy]ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



RN 678992-82-0 CAPLUS

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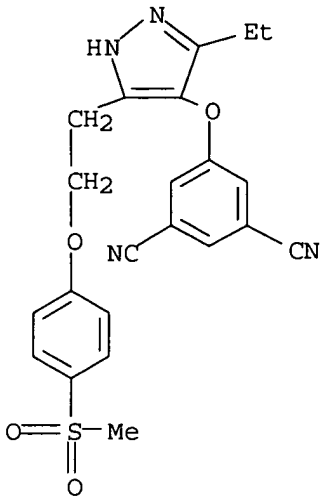

RN 678992-85-3 CAPLUS
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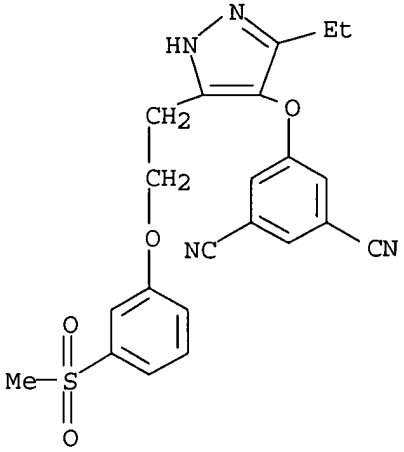
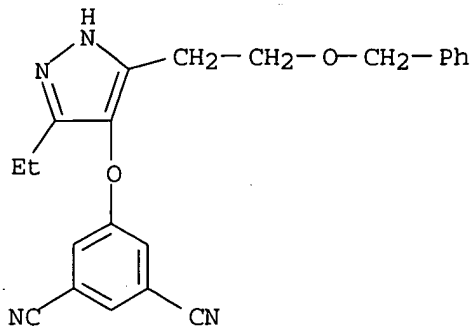


IT **473921-46-9P 473921-47-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazole derivs. as therapeutic agents for HIV mediated diseases)
RN 473921-46-9 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-(phenylmethoxy)ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



RN 473921-47-0 CAPLUS
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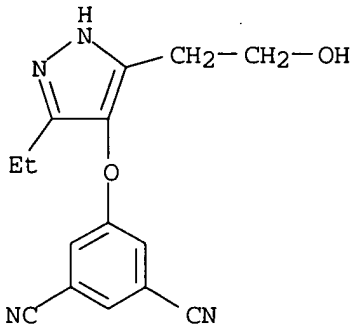

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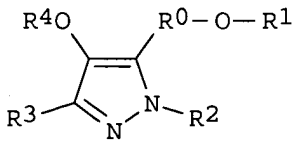

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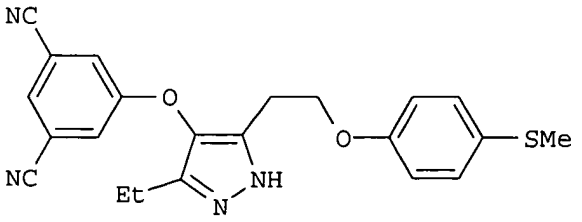


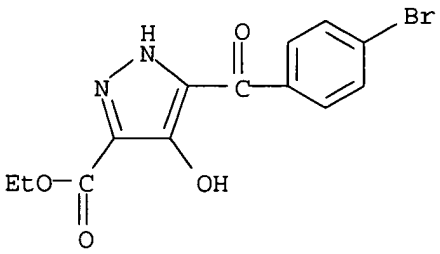
II

AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are

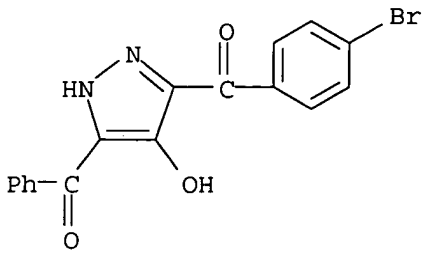
useful in the treatment of a variety of disorders including those in which the inhibition' of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodificiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-{[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

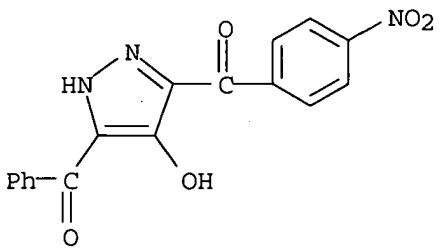
L22 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:63587 CAPLUS
DOCUMENT NUMBER: 141:243399
TITLE: Chemistry of Diazopolycarbonyl Compounds: VIII. Synthesis of Nitrogen-containing Heterocycles via Transformations of Substituted 2-diazopentane-1,3,5-triones
AUTHOR(S): Kutkovaya, N. V.; Vyaznikova, N. G.; Zalesov, V. V.
CORPORATE SOURCE: Research Institute of Vaccines and Serum at Federal State Unitary Enterprise "Biomed", Perm, Russia
SOURCE: Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2003), 39(11), 1644-1648
CODEN: RJOCEQ; ISSN: 1070-4280
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:243399
IT **749923-98-6P 749923-99-7P 749924-00-3P 749924-01-4P 749924-02-5P 749924-03-6P 749924-04-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of nitrogen-containing heterocycles via transformations of substituted diazopentanetriones)
RN 749923-98-6 CAPLUS
CN 1H-Pyrazole-3-carboxylic acid, 5-(4-bromobenzoyl)-4-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)



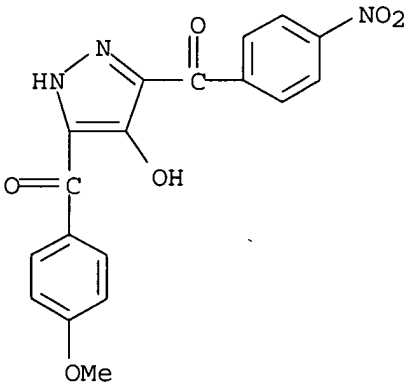
RN 749923-99-7 CAPLUS
CN Methanone, (5-benzoyl-4-hydroxy-1H-pyrazol-3-yl)(4-bromophenyl)- (9CI) (CA INDEX NAME)



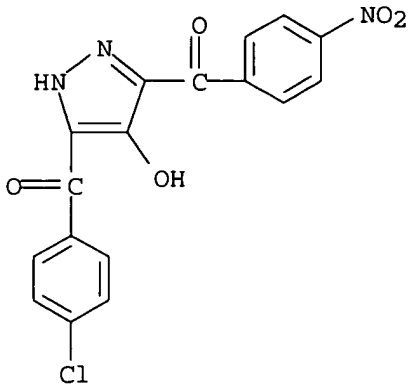
RN 749924-00-3 CAPLUS
CN Methanone, (5-benzoyl-4-hydroxy-1H-pyrazol-3-yl)(4-nitrophenyl)- (9CI) (CA INDEX NAME)



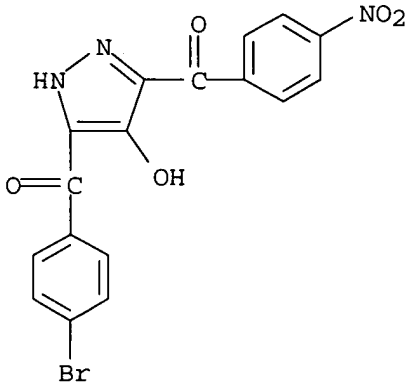
RN 749924-01-4 CAPLUS
CN Methanone, [4-hydroxy-5-(4-methoxybenzoyl)-1H-pyrazol-3-yl](4-nitrophenyl)- (9CI) (CA INDEX NAME)



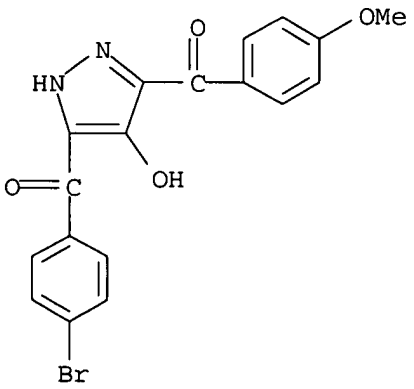
RN 749924-02-5 CAPLUS
CN Methanone, [5-(4-chlorobenzoyl)-4-hydroxy-1H-pyrazol-3-yl](4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 749924-03-6 CAPLUS
CN Methanone, [5-(4-bromobenzoyl)-4-hydroxy-1H-pyrazol-3-yl](4-nitrophenyl)-
(9CI) (CA INDEX NAME)



RN 749924-04-7 CAPLUS
CN Methanone, [5-(4-bromobenzoyl)-4-hydroxy-1H-pyrazol-3-yl](4-methoxyphenyl)-
(9CI) (CA INDEX NAME)



AB Et 5-aryl-2-diazo-3,5-dioxopentanoates and 1,5-diaryl-2-diazopentane-1,3,5-triones are partially enolized in solns. By O-methylation of enol forms of diazo esters with diazomethane Et 5-aryl-2-diazo-5-methoxy-3-oxopent-4-enoates were prepared Concurrently with the O-methylation the diazo esters undergo heterocyclization into 3,5-disubstituted 4-hydroxypyrazoles which under the reaction condition suffer O- and N-methylation by excess diazomethane. 3,5-Diaroyl-4-hydroxypyrazoles were also obtained from diazopentanetriones but here triethylamine served as the cyclization reagent.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

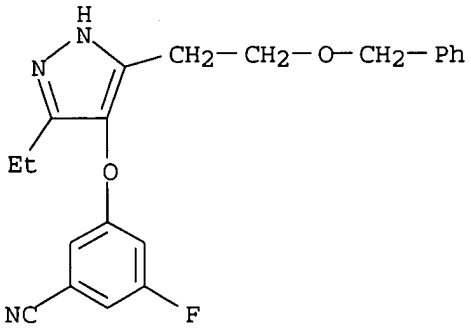
L22 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:832763 CAPLUS
DOCUMENT NUMBER: 137:337884
TITLE: Preparation of aryloxy pyrazole derivatives as reverse transcriptase inhibitors for treating HIV
INVENTOR(S): Jones, Lyn Howard; Mowbray, Charles Eric; Price, Davis Anthony; Selby, Matthew Duncan; Stupple, Paul Anthony
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002085860	A1	20021031	WO 2002-IB1234		20020404
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2443449	AA	20021031	CA 2002-2443449		20020404
EP 1377556	A1	20040107	EP 2002-708600		20020404
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
EE 200300497	A	20040216	EE 2003-497		20020404
BR 2002008811	A	20040309	BR 2002-8811		20020404
JP 2004531535	T2	20041014	JP 2002-583387		20020404
US 2003100554	A1	20030529	US 2002-118512		20020405
ZA 2003007095	A	20040910	ZA 2003-7095		20030910
NO 2003004523	A	20031209	NO 2003-4523		20031009
PRIORITY APPLN. INFO.:			GB 2001-8999	A	20010410
			GB 2001-27426	A	20011115
			US 2001-289570P	P	20010508
			US 2002-346727P	P	20020107
			WO 2002-IB1234	W	20020404

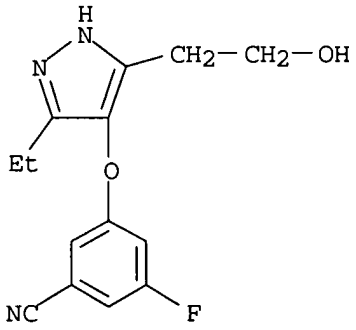
OTHER SOURCE(S): MARPAT 137:337884
IT **473921-40-3P**, 3-[[5-[2-(Benzyloxy)ethyl]-3-ethyl-1H-pyrazol-4-

yl]oxy]-5-fluorobenzonitrile **473921-41-4P**, 3-[[3-Ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]-5-fluorobenzonitrile **473921-46-9P**, 5-[[5-[2-(Benzyloxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]isophthalonitrile
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)

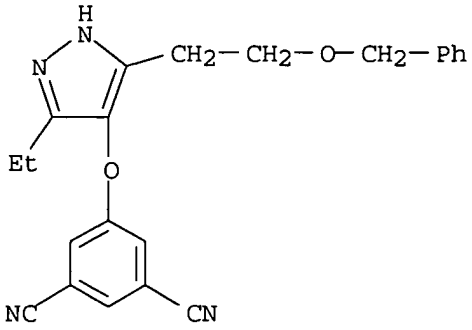
RN 473921-40-3 CAPLUS
CN Benzonitrile, 3-[[3-ethyl-5-[2-(phenylmethoxy)ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 473921-41-4 CAPLUS
CN Benzonitrile, 3-[[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



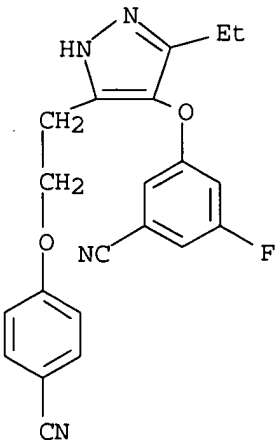
RN 473921-46-9 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-[2-(phenylmethoxy)ethyl]-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



IT **473921-42-5P**, 3-[[5-[2-(4-Cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluorobenzonitrile **473921-43-6P**, 3-Fluoro-5-[[3-ethyl-5-(2-((2-methyl-3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile **473921-44-7P**, 3-Fluoro-5-[[3-ethyl-5-(2-((3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile **473921-45-8P**, 3-Fluoro-5-[[3-ethyl-5-(2-((2-amino-3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile **473921-47-0P**, 5-[[3-Ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]isophthalonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)

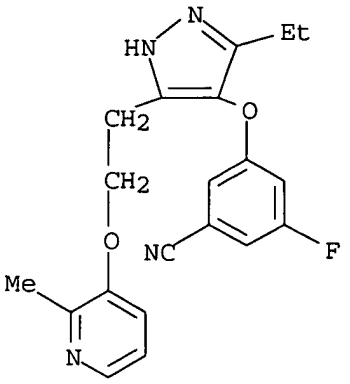
RN 473921-42-5 CAPLUS

CN Benzonitrile, 3-[[5-[2-(4-cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)

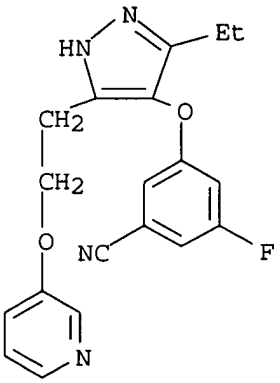


RN 473921-43-6 CAPLUS

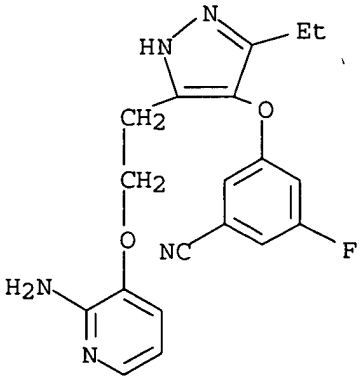
CN Benzonitrile, 3-[[3-ethyl-5-[2-[(2-methyl-3-pyridinyl)oxy]ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



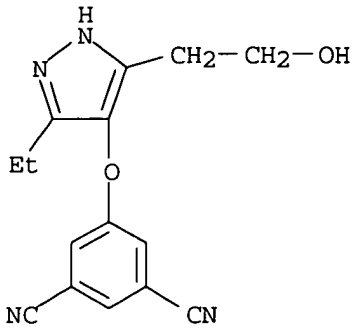
RN 473921-44-7 CAPLUS
CN Benzonitrile, 3-[[3-ethyl-5-[2-(3-pyridinyloxy)ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 473921-45-8 CAPLUS
CN Benzonitrile, 3-[[5-[2-[(2-amino-3-pyridinyl)oxy]ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 473921-47-0 CAPLUS
CN 1,3-Benzenedicarbonitrile, 5-[[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]- (9CI) (CA INDEX NAME)



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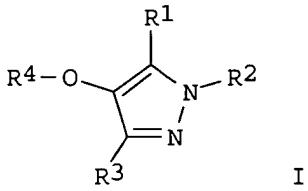


I

AB This invention relates to pyrazole derivs. (shown as I; e.g. 2-Amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone) or pharmaceutically acceptable salts, solvates or derivative thereof, wherein R1 to R4 are defined below, and to processes for the preparation thereof, intermediates used in their preparation of, compns. containing them and the uses of such derivs. The compds. of the present invention bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof. As such the compds. of the present invention are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). In tests of inhibition of HIV-1 reverse transcriptase enzyme, the claimed compds. 2-amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone, 3,5-dimethyl-4-[[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]benzonitrile and 1-(3-azetidinyl)-4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazole had IC50 values of 39,000, 3,200 and 248 nM, resp. In I: R1 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R10, -CONR5R10, R8 or R9. R2 is H, C1-C6 alkyl, C3-C6 alkenyl, C3-C6 alkynyl, C3-C7 cycloalkyl, C3-C7 cycloalkenyl, Ph, benzyl, R8 or R9; or, R1 and R2, when taken together, represent unbranched C3-C4 alkylene. R3 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R5, -CONR5R5, R8 or R9; R4 is Ph, naphthyl or pyridyl. Definitions of R5 and R7-R10 and addnl. specifications are given in the claims. Included are 283 claimed-compound prepns. and 115 intermediate prepns.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:375284 CAPLUS
DOCUMENT NUMBER: 131:31936
TITLE: Selective β3 adrenergic agonists
INVENTOR(S): Crowell, Thomas Alan; Jones, Charles David; Shuker, Anthony John
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: Eur. Pat. Appl., 48 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

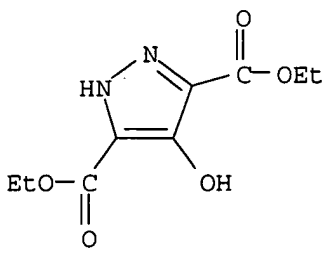
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 921120	A1	19990609	EP 1998-309868	19981202
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
ZA 9811026	A	20000602	ZA 1998-11026	19981202
CA 2312987	AA	19990617	CA 1998-2312987	19981204
WO 9929673	A1	19990617	WO 1998-US25831	19981204
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9916281	A1	19990628	AU 1999-16281	19981204
US 6046227	A	20000404	US 1998-206107	19981204
JP 2001525399	T2	20011211	JP 2000-524270	19981204
US 6617347	B1	20030909	US 1999-443272	19991118

PRIORITY APPLN. INFO.:
US 1997-67599P P 19971205
US 1998-204372 A1 19981202
US 1998-206107 A3 19981204
WO 1998-US25831 W 19981204

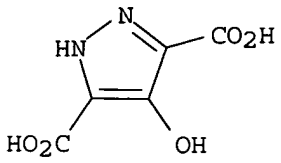
OTHER SOURCE(S): MARPAT 131:31936

IT **23705-86-4P 226989-47-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pyrazole derivs. as selective β3 adrenergic agonists)

RN 23705-86-4 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



RN 226989-47-5 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy- (9CI) (CA INDEX NAME)



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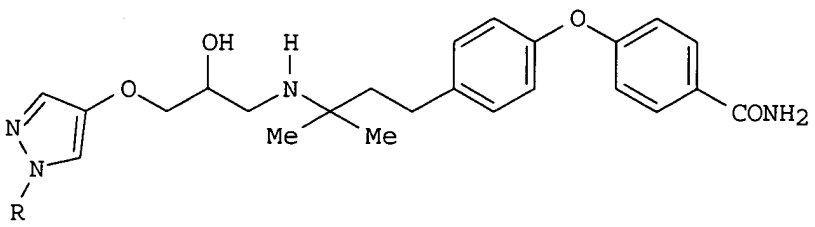
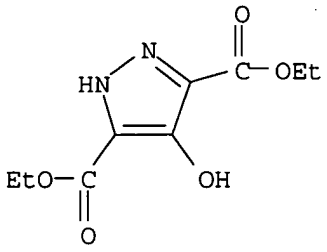


I

AB Pyrazole derivs. such as I (R = H) were prepared as β3 adrenergic agonists. Thus, 1.75 g (S)-1-benzyl-4-glycidylpyrazole and 3.6 g 4-Me2C(NH2)CH2CH2C6H4OC6H4CONH2-4 were heated to 45° for 72 h in 100 mL EtOH to give I (R = benzyl) in 52.5% yield. Hydrogenolysis of I (benzyl) over 20% Pd(OH)2/C in EtOH at 40° for 72 h gave I (R = H) in 32% yield. A combinatorial chemical example was also given. In evaluating β3 agonist activity (cAMP assays), the present compds. showed at least 30%, preferably 50%, and most preferably >85% of isoproterenol's response at a single dose of 50 mmol.
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:162019 CAPLUS
DOCUMENT NUMBER: 130:237515
TITLE: Selective dopamine receptors: synthesis, complexing properties, and molecular modeling studies of new podands derived from 4-hydroxy-1H-pyrazole
AUTHOR(S): Rodriguez-Franco, Maria Isabel; San Lorenzo, Patricia; Martinez, Ana; Navarro, Pilar
CORPORATE SOURCE: Instituto de Quimica Medica (C.S.I.C.), Madrid, 28006, Spain
SOURCE: Tetrahedron (1999), 55(9), 2763-2772
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:237515
IT **23705-86-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of hydroxypyrazole podands, mol. modeling, and complexation behavior toward cations and dopamine and norepinephrine)
RN 23705-86-4 CAPLUS

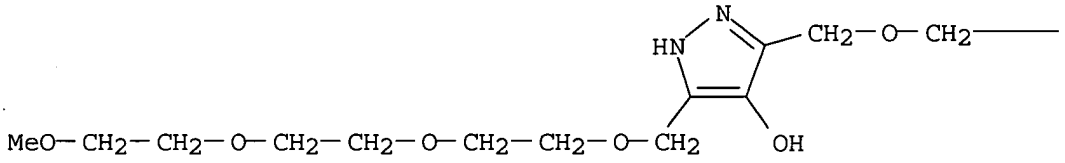
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



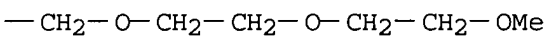
IT **221347-44-0P 221347-45-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hydroxypyrazole podands, mol. modeling, and complexation behavior toward cations and dopamine and norepinephrine)

RN 221347-44-0 CAPLUS
CN 1H-Pyrazol-4-ol, 3,5-bis(2,5,8,11-tetraoxadodec-1-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A

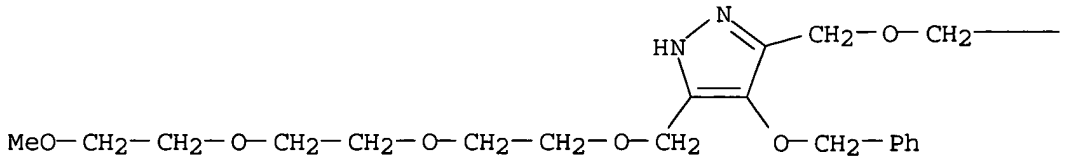


PAGE 1-B

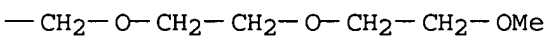


RN 221347-45-1 CAPLUS
CN 1H-Pyrazole, 4-(phenylmethoxy)-3,5-bis(2,5,8,11-tetraoxadodec-1-yl)- (9CI) (CA INDEX NAME)

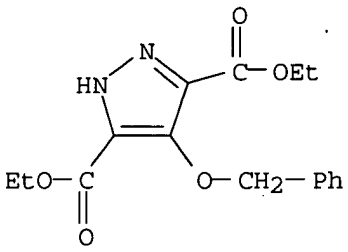
PAGE 1-A



PAGE 1-B



IT **221347-37-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of hydroxypyrazole podands, mol. modeling, and complexation behavior toward cations and dopamine and norepinephrine)
RN 221347-37-1 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-(phenylmethoxy)-, diethyl ester (9CI) (CA INDEX NAME)



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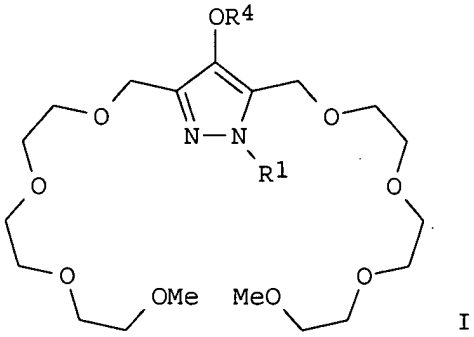


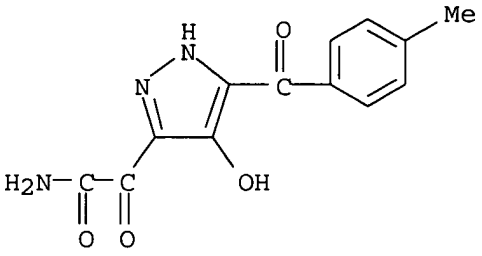
I

AB New podands, I (R1 = R4 = CH2Ph, H; R1 = CH2Ph, R4 = H; R1 = H, R4 = CH2Ph), derived from 4-hydroxy-1H-pyrazole have been prepared Their complexing properties toward cations (Na+, K+, NH4+) and some neurotransmitters (dopamine and norepinephrine) have been studied, using biphasic extraction expts., mol. modeling, and a NMR titration Podand I (R1 = CH2Ph, R4 = H), 1-benzyl-4-hydroxy-3,5-bis(2,5,8,11-tetraoxadodecan-1-yl)-1H-pyrazole, showed an interesting selective complexation of dopamine.
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:162161 CAPLUS
DOCUMENT NUMBER: 124:317104
TITLE: Chemistry of diazopolycarbonyl compounds. II. Synthesis of aroylacetyl derivatives of diazopyruvic acid esters and their reaction with ammonia and o-phenylenediamine
AUTHOR(S): Zalesov, V. V.; Vyaznikova, N. G.; Andreichikov, Yu. S.
CORPORATE SOURCE: Perm. Farm. Inst., Russia

SOURCE: Zhurnal Organicheskoi Khimii (1995), 31(8), 1213-17
CODEN: ZORKAE; ISSN: 0514-7492
PUBLISHER: Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian

IT **176375-05-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 176375-05-6 CAPLUS
CN 1H-Pyrazole-3-acetamide, 4-hydroxy-5-(4-methylbenzoyl)-α-oxo- (9CI)
(CA INDEX NAME)



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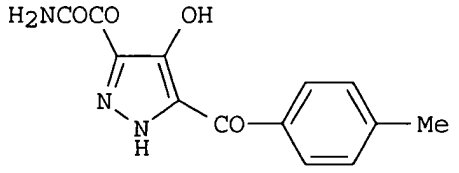

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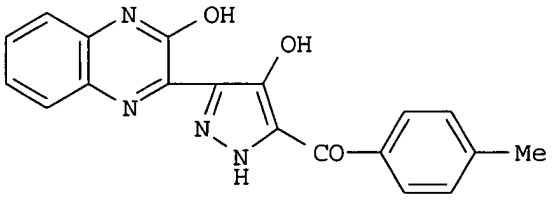
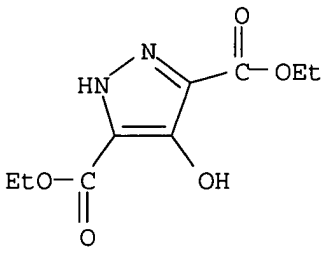


III

AB (Z)-R1OCOCOC(:N2)COCH:C(OH)C6H4R2-4 (I; R1 = Et, Pr, Bu; R2 = H, Me, OMe, Cl, Br) were prepared by reaction of 5-aryl-2,3-furandiones with R1OCOCOCHN2. Reaction of I with NH4OH gave pyrazoles, e.g., II, and reaction with o-phenylenediamine gave pyrazolylquinoxalines, e.g., III. Other quinoxalines were prepared from the arylfurandiones and o-phenylenediamine.

L22 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:89704 CAPLUS
DOCUMENT NUMBER: 86:89704
TITLE: Synthesis and biological activity of 1,2,3-triazolo-1,8-naphthyridine derivatives

AUTHOR(S): Livi, O.; Ferrarini, P. L.; Tonetti, I.
CORPORATE SOURCE: Ist. Chim. Farm., Univ. Pisa, Pisa, Italy
SOURCE: Farmaco, Edizione Scientifica (1976), 31(11), 797-808
CODEN: FRPSAX; ISSN: 0430-0920
DOCUMENT TYPE: Journal
LANGUAGE: Italian
OTHER SOURCE(S): CASREACT 86:89704
IT **23705-86-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23705-86-4 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



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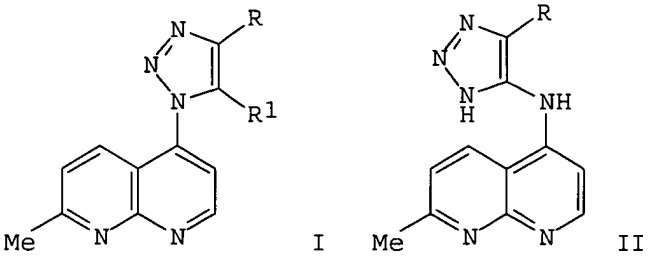


AB Triazolylnaphthyridines I (R = Ph, CO2Et, cyano, R1 = NH2; R = CO2Et, CO2H, R1 = Me, Ph, 4-O2NC6H4; R = Ac, Bz, R1 = Me, Ph; R = Ph, CONHPh, R1 = Me; R = CO2Et, R1 = CH2CO2Et; R = H, R1 = 4-O2NC6H4) were prepared by reaction of 2-methyl-5-azido-1,8-naphthyridine with RCH2CN or RCOCH2R1. I (R1 = NH2) rearranged on heating to the triazolylaminonaphthyridines II. I (R = CONHPh, R1 = Me) had twice the analgesic activity of phenylbutazone. I (R = Ac, Ph, R1 = Me) and II (R = Ph) had sedative activity (no data) and II (R = Ph, CO2H) were fungicidal.

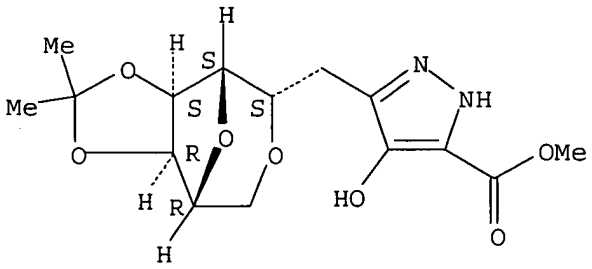
L22 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:43964 CAPLUS
DOCUMENT NUMBER: 86:43964
TITLE: Syntheses of C-nucleosides. IX. Reactions of D,L-3,4-di-O-isopropylidene-2,5-anhydroallose with Wittig reagents. Syntheses of bis-homo anhydro-C-nucleosides
AUTHOR(S): Just, George; Ramjeesingh, Mohabir; Liak, Teng Jiam
CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, Can.

SOURCE: Canadian Journal of Chemistry (1976), 54(18), 2940-7
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English

IT **61407-36-1P 61407-37-2P 61407-38-3P**
61407-39-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

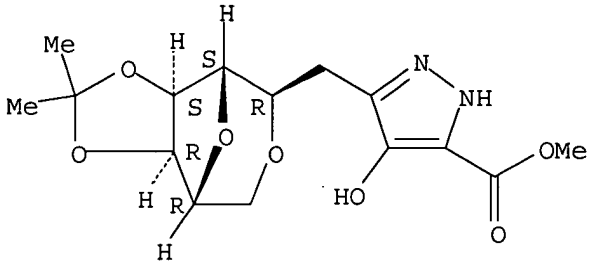
RN 61407-36-1 CAPLUS
CN D-glycero-D-allo-Heptitol, 2,7:3,6-dianhydro-1-deoxy-1-[4-hydroxy-5-(methoxycarbonyl)-1H-pyrazol-3-yl]-4,5-O-(1-methylethylidene)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



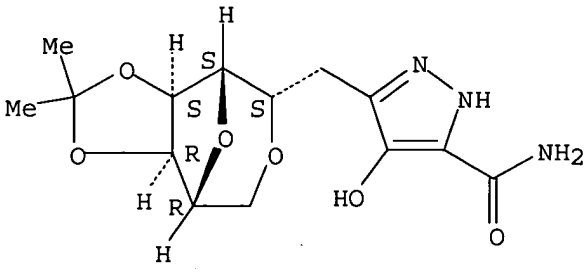
RN 61407-37-2 CAPLUS
CN D-glycero-D-altro-Heptitol, 2,7:3,6-dianhydro-1-deoxy-1-[4-hydroxy-5-(methoxycarbonyl)-1H-pyrazol-3-yl]-4,5-O-(1-methylethylidene)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



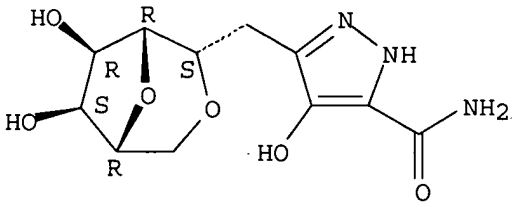
RN 61407-38-3 CAPLUS
CN D-glycero-D-allo-Heptitol, 1-[5-(aminocarbonyl)-4-hydroxy-1H-pyrazol-3-yl]-2,7:3,6-dianhydro-1-deoxy-4,5-O-(1-methylethylidene)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 61407-39-4 CAPLUS
CN D-glycero-D-allo-Heptitol, 1-[5-(aminocarbonyl)-4-hydroxy-1H-pyrazol-3-yl]-2,7:3,6-dianhydro-1-deoxy-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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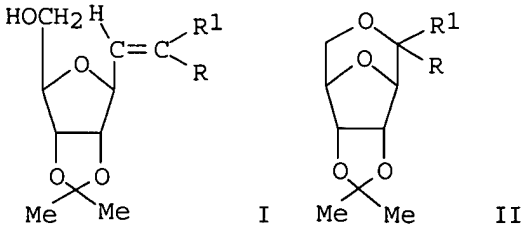


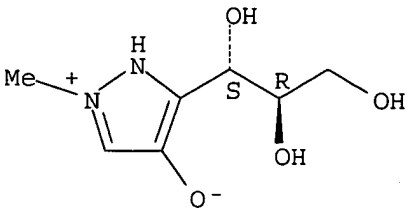
I II

AB The NMR spectra of the two anomers of 1-O-acetyl-3,4-di-O-isopropylidene-2,5-anhydro-D,L-allose are discussed. Wittig reactions of D,L-3,4-di-O-isopropylidene-2,5-anhydroallose gave the olefins I (R = H, R1 = CO2Et; R = Br, R1 = CO2Et; R = CO2Et, R1 = Br; R = H, R1 = COCO2Et) and an internal Michael addition product II (R = H, R1 = CH2COCO2Et; R = CH2COCO2Et, R1 = H). II gave two bis-homo anhydro-C-nucleosides having 6-azauracil and 4-hydroxy-5-carboxamidopyrazole base.

L22 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1970:445752 CAPLUS
DOCUMENT NUMBER: 73:45752
TITLE: Hydrazine reactions. XII. Reaction of 4-ulose hydrazones to 4-hydroxypyridazines and of 3-ulose hydrazones to 4-hydroxypyrazoles
AUTHOR(S): Paulsen, Hans; Steinert, Karin; Steinert, Gerd
CORPORATE SOURCE: Inst. Org. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1970), 103(6), 1846-54

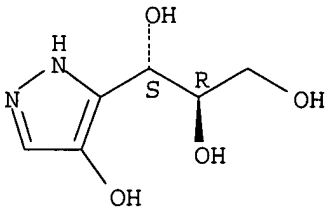
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 73:45752
IT **29673-22-1P 29906-02-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29673-22-1 CAPLUS
CN Pyrazolium, 4-hydroxy-2-methyl-5-(D-erythro-1,2,3-trihydroxypropyl)-, hydroxide, inner salt (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 29906-02-3 CAPLUS
CN 1,2,3-Propanetriol, 1-(4-hydroxypyrazol-3-yl)-, D-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



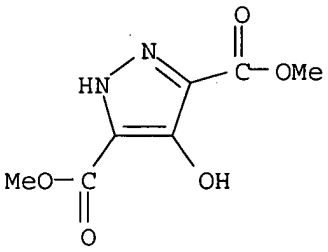
GI For diagram(s), see printed CA Issue.
AB 2,3:5,6-Di-O-isopropylidene-D-xylo-hexos-4-ulose hydrazone di-Me acetal was cyclized with 2N HCl to give (via the corresponding 1:1 4- and 5-hydroxypyridazinium chloride, with subsequent HCl cleavage) 3-(D-glycero-1,2-dihydroxyethyl)-4(1H)- and -5(2H)-pyridazinone (I and II). The corresponding N'-methylhydrazone gave only the 5-hydroxy derivative, isolated as a zwitterion. 3,5-Dideoxy-3-hydrazino-1,2-O-isopropylidene-D-ribofuranose p-toluenesulfonate, prepared from 5-deoxy-1,2-O-isopropylidene-3-O-p-tolylsulfonyl-D-xylofuranose and H2NNH2, gave with 2N HCl 5-(D-glycero-1-hydroxyethyl)pyrazole (III, R = Me). Similarly, 1,2:5,6-Di-O-isopropylidene-α-D-ribo-hexofuranos-3-ulose hydrazone gave 4-hydroxy-5-(D-erythro-1,2,3-trihydroxypropyl)pyrazole [III, R = CH(OH)CH2OH]. NMR and uv data were reported.

L22 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1969:47359 CAPLUS
DOCUMENT NUMBER: 70:47359
TITLE: Esters of 4-hydroxypyrazole-3,5-dicarboxylic acid
AUTHOR(S): Begtrup, Mikael; Larsen, P. Skov; Pedersen, Christian
CORPORATE SOURCE: Org.-Kem. Lab., Polytek. Laereanstalt, Lyngby, Den.
SOURCE: Acta Chemica Scandinavica (1947-1973) (1968), 22(8), 2476-8

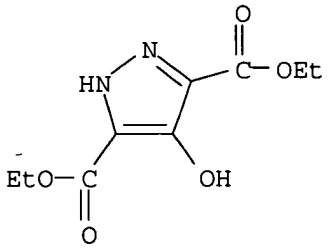
CODEN: ACSAA4; ISSN: 0001-5393
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 70:47359

IT **23705-85-3P 23705-86-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23705-85-3 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, dimethyl ester (9CI) (CA INDEX NAME)



RN 23705-86-4 CAPLUS
CN 1H-Pyrazole-3,5-dicarboxylic acid, 4-hydroxy-, diethyl ester (9CI) (CA INDEX NAME)



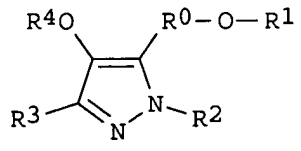
AB The base catalyzed reaction of di-Me diazomalonate with di-Me malonate (I) gives a high yield of di-Me 4-hydroxypyrazole-3,5-dicarboxylate (II). The corresponding di-Et ester was obtained in low yield only. The mechanism of the formation of II as a by-product in the reaction of PhN3 with I is discussed.

=> log y

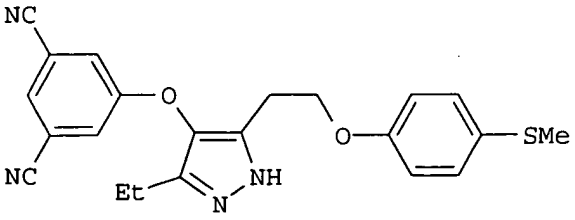
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	119.46	961.80

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-17.52	-21.17

STN INTERNATIONAL LOGOFF AT 19:26:04 ON 15 APR 2005



I



II

AB The title compds. [I; R0 = absent, alkylene; R1 = Ph substituted by SOyR5, alkylene(SOyR5), SOyCF3, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, cycloalkyl, Ph, etc.; R4 = (un)substituted Ph, naphthyl, pyridyl; R5 = H, alkyl, cycloalkyl, etc.; y = 0-2] which bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof, and as such are useful in the treatment of a variety of disorders including those in which the inhibition' of reverse transcriptase is implicated, were prepared and formulated. Disorders of interest include those caused by Human Immunodificiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). Thus, reacting 5-{[3-ethyl-5-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy}isophthalonitrile (preparation given) with 4-(methylmercapto)phenol afforded I [R0 = (CH2)2; R1 = 4-(MeS)C6H4; R2 = H; R3 = Et; R4 = 3,5-(NC)2C6H3] which showed IC50 of 2 nM against HIV-1 reverse transcriptase. The pharmaceutical composition comprising the compound I is claimed.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l14 ibib hitstr abs 2

L14 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:832763 CAPLUS
DOCUMENT NUMBER: 137:337884
TITLE: Preparation of aryloxy pyrazole derivatives as reverse transcriptase inhibitors for treating HIV
INVENTOR(S): Jones, Lyn Howard; Mowbray, Charles Eric; Price, Davis Anthony; Selby, Matthew Duncan; Stupple, Paul Anthony
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
SOURCE: PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085860	A1	20021031	WO 2002-IB1234	20020404

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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EP 1377556	A1	20040107	EP 2002-708600	20020404
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ZA 2003007095	A	20040910	ZA 2003-7095	~~20030910~~
NO 2003004523	A	20031209	NO 2003-4523	20031009
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			GB 2001-27426	A 20011115
			US 2001-289570P	P 20010508
			US 2002-346727P	P 20020107
			WO 2002-IB1234	W 20020404

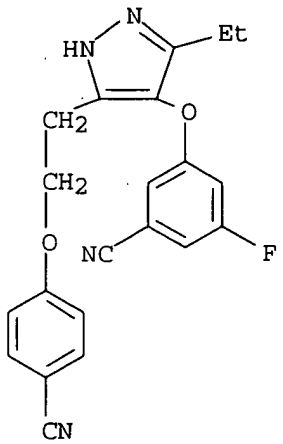
Allowed

OTHER SOURCE(S): MARPAT 137:337884

IT **473921-42-5P**, 3-[[5-[2-(4-Cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluorobenzonitrile **473921-43-6P**, 3-Fluoro-5-[[3-ethyl-5-(2-((2-methyl-3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile **473921-44-7P**, 3-Fluoro-5-[[3-ethyl-5-(2-((3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile **473921-45-8P**, 3-Fluoro-5-[[3-ethyl-5-(2-((2-amino-3-pyridyl)oxy)ethyl)-1H-pyrazol-4-yl]oxy]benzonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aryloxy pyrazole derivs. as reverse transcriptase inhibitors for treating HIV)

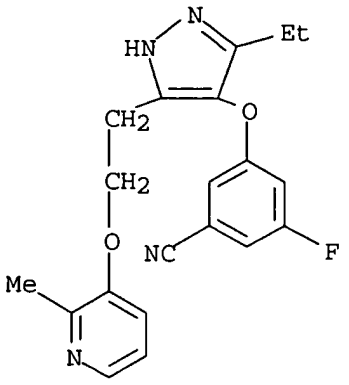
RN 473921-42-5 CAPLUS

CN Benzonitrile, 3-[[5-[2-(4-cyanophenoxy)ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)

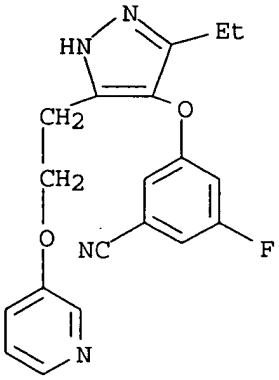


RN 473921-43-6 CAPLUS

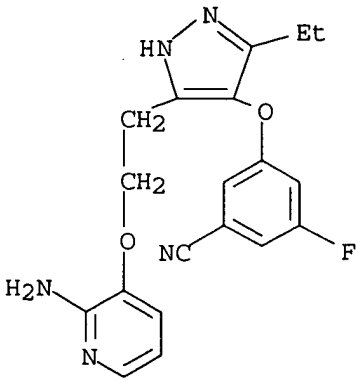
CN Benzonitrile, 3-[[3-ethyl-5-[2-[(2-methyl-3-pyridinyl)oxy]ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



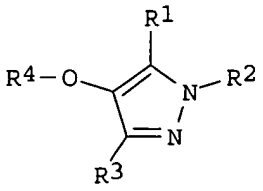
RN 473921-44-7 CAPLUS
CN Benzonitrile, 3-[[3-ethyl-5-[2-(3-pyridinyloxy)ethyl]-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 473921-45-8 CAPLUS
CN Benzonitrile, 3-[[5-[2-[(2-amino-3-pyridinyl)oxy]ethyl]-3-ethyl-1H-pyrazol-4-yl]oxy]-5-fluoro- (9CI) (CA INDEX NAME)



GI



I

AB This invention relates to pyrazole derivs. (shown as I; e.g. 2-Amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone) or pharmaceutically acceptable salts, solvates or derivative thereof, wherein R1 to R4 are defined below, and to processes for the preparation thereof, intermediates used in their preparation of, compns. containing them and the uses of such derivs. The compds. of the present invention bind to the enzyme reverse transcriptase and are modulators, especially inhibitors thereof. As such the compds. of the present invention are useful in the treatment of a variety of disorders including those in which the inhibition of reverse transcriptase is implicated. Disorders of interest include those caused by Human Immunodeficiency Virus (HIV) and genetically related retroviruses, such as Acquired Immune Deficiency Syndrome (AIDS). In tests of inhibition of HIV-1 reverse transcriptase enzyme, the claimed compds. 2-amino-6-[[4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazol-1-yl]methyl]-4(3H)-pyrimidinone, 3,5-dimethyl-4-[[3,5-diethyl-1-(2-hydroxyethyl)-1H-pyrazol-4-yl]oxy]benzonitrile and 1-(3-azetidinyl)-4-(3,5-dichlorophenoxy)-3,5-diethyl-1H-pyrazole had IC50 values of 39,000, 3,200 and 248 nM, resp. In I: R1 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R10, -CONR5R10, R8 or R9. R2 is H, C1-C6 alkyl, C3-C6 alkenyl, C3-C6 alkynyl, C3-C7 cycloalkyl, C3-C7 cycloalkenyl, Ph, benzyl, R8 or R9; or, R1 and R2, when taken together, represent unbranched C3-C4 alkylene. R3 is H, C1-C6 alkyl, C3-C7 cycloalkyl, Ph, benzyl, halo, -CN, -OR7, -CO2R5, -CONR5R5, R8 or R9; R4 is Ph, naphthyl or pyridyl. Definitions of R5 and R7-R10 and addnl. specifications are given in the claims. Included are 283 claimed-compound prepns. and 115 intermediate prepns.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	12.58	516.53

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.46	-3.65

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